United States Army
FRANKFORD ARSENAL
Philadelphia, Pa., 19137

ADDRESS REPLY TO
COMMANDING OFFICER
FRANKFORD ARSENAL
ATTN:

SMUFA - 1312
S. H. EISMAN

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Prof. Joshua Lederberg
Stanford University
Medical Center
Department of Genetics
Palo Alto, California

Dear Prof. Lederberg:

I want to thank you for your very kind letter and the notes which you sent me on October 28. I'm terribly sorry for taking so long in replying.

It was interesting to see that you were using parts of an Algol translator for processing non-cyclic molecular structures. My own background is in computer applications and I arrived at this linear notation in the same fashion by reinterpreting the tree forms generated by arithmetic expressions.

The generation of a canonical representation seems to be a most difficult problem for cyclic structures. For trees, I believe the notion of a center goes back to Cayley and, although I don't remember the exact reference, I think it was his second or third paper on the subject. Neville, in Proc. Camb. Phil. Soc. V 49, 1953 has an interesting paper on codifying trees. As far as more general structures are concerned, Gluck (DuPont) reported on an early attempt at the Spring, 1964 meeting of the ACS. This method was shown to be incorrect (by Dr. Alfred Lehman, Walter Reed Army Institute for Research) with the 'bipentagon' serving as the counterexample. More recently, I have heard that Gluck and Cossum (of Chem. Abstracts) have a procedure for generating a canonical representation of an arbitrary graph and that it has been 'proven mathematically to be a valid one' by a Dr. Pepper of Ohio State Univ. I have not seen this proof but it has been described to me as occupying twenty-five, doubly spaced typewritten pages.

Dr. Lehman is looking into canonical forms and I believe he may have something for planar graphs but I am not certain. So far, he can do nothing with non-planar graphs. I believe Lehman might be a good person to get in touch with since he is quite knowledgeable in this area.

I have several questions about the paper "Topological Mappings of Organic Molecules". If I understand you correctly you are suggesting an orderly generation of polyhedra from which polygonal graphs can be determined which in turn will lead to various ring structures. I have trouble visualizing three dimensional figures (particularly 8C of Fig. 1) much less ordering them and prefer looking at the polygonal structures for generating and ordering the cubical graphs. And what I am really doing, I find, is not looking at geometrical figures at all but listing connections of nodes in a systematic fashion. The polyhedra certainly seem more practical for recognizing isomorphisms but the polygons seem more useful otherwise. (There appear to be some extra edges in 10B and 10C and I couldn't resolve those two figures)

Also, the polygons don't map into a single ring structure. For example, 8F (Fig. 2) may represent RRI 6310 or 6128; 8L 6376, 6377 or several others. The size of the rings is not specified either so again there is ambiguity. Giving weights to the branches might circumvent the first difficulty and specifying ring sizes would alleviate the second.

I don't feel non-planar graphs should be discarded. In addition to catenanes, knotted structures have been suggested as possibilities and, even though it doesn't prove anything, there's at least one chemist who has built models of non-planar structures and claims he could synthesize them if he wanted to.

The polycene notation scheme is quite interesting and should be of some use. I tried handling fused rings, at first, by considering them as nodes connected to each other by multivalent bonds - using the notion of lists to make up larger and larger units. This failed rather quickly when we got to rings of rings (e.g. ovalene). I wonder if other than 6-membered rings could be handled in the polycene system if they are surrounded by many other rings. If the odd rings are not deeply embedded they could just be labelled with their sizes but otherwise they would distort the mosaic.

There is a paper by R. Tabory in "Symbolic Languages in Data Processing" (Gordon & Breach) which is concerned with a language for constructing and manipulating graphs. This may be of interest to the computer people who are working with this problem.

Sincerely yours,

S. H. EISMAN